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Strongly Interacting Fermi Gases of Atoms Confined in a Harmonic Trap

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Dynamics of strongly interacting Fermi gases, consisting of a 50-50 mixture of two different fermionic species, is investigated. For the equation of state we consider a Padé [2/2] approximations, which gives the weak-coupling perturbative formula (up to 4th order) in the low density regime, the unitary-limit Monte Carlo result in the high density regime, and reproduces the 4-fermion prediction for dimer-dimer scattering length in the BEC region. We use a time-dependent LDA to derive various properties of the Fermi gas under a harmonic confinement and compare them with the data of very recent experiments of ^6Li atoms across a Feshbach resonance.

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In this talk the dynamics of strongly interacting dilute Fermi gases (dilute in the sense that the range of interatomic potential is small compared with inter-particle spacing) consisting of a 50-50 mixture of two different states and confined in a harmonic trap $V_{ext}(\vec{r}) = (m/2)(\omega_\perp^2(x^2+y^2)+\omega_z^2 z^2)$ is investigated in the single equation approach to the time-dependent density-functional theory [1,2]

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V_{ext}\Psi + V_{xc}\Psi, \tag{1}$$

where $V_{xc}(\vec{r},t) = [\frac{\partial n\epsilon(n)}{\partial n}]_{n=n(\vec{r},t)}$, the density of the system is $n(\vec{r},t) = \mid \Psi(\vec{r},t) \mid^2$, and the velocity field $\vec{\mathrm{v}}(\vec{r},t) = \hbar(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*)/(2imn(\vec{r},t))$.

Let us come back to the variational formulation of the Kohn-Sham time-dependent theory

$$\delta\int dt < \psi|i\hbar\partial_t - H|\psi >, \tag{2}$$

where $|\psi>$ is a product of two Slater determinants, one for each internal state built up by the Kohn-Sham orbitals ψ_i, and $H = T + U$ is the LDA Hamiltonian.

Eq.(1) can be derived from Eq.(2) using two approximations

(i) local transform $\psi_i \approx \phi_i \exp(i\hbar\chi/m)$, where ψ_i and χ are real functions,

and

(ii) $<\phi|T|\phi> \approx \int(t_{TF}(n) + t_W(n))n(\vec{r},t)d^3r$,

where $|\phi>$ is the product of two Slater determinants built on ϕ_i alone, $t_{TF}(n) = (3\pi^2)^{2/3}(3\hbar^2/(10m))n(\vec{r},t)^{2/3}$ is the Thomas-Fermi kinetic energy density, and $t_W(n) = (\hbar^2/(8m))(\nabla n)^2/n$ is the original von Weizsäcker density (OWD).

We note here that the approximations (i) and $<\phi|T|\phi> \approx \int t_{TF}(n)n(\vec{r},t)d^3r$ lead to the hydrodynamic approximation (HA) [3]. But near the surface the Hartree-Fock (HF) type densities are proportional to the square of the last occupied state. Therefore, the OWD is important in this case and it is expected to determine the asymptotic behavior of the density at large distances. It is also expected that the OWD is important in the case of the tight radial trapping, $\lambda \ll 1$.

Taking into account that in the limit $a \to -0$, where a is the scattering length, Eq.(2) leads to exact equations describing scaling properties of a ideal gas trapped in a time-dependent harmonic potential [4], we do expect that the Kohn-Sham approach may be an appropriate to describe dynamics of cold fermionic gas in the regime when superfluid quantum hydrodynamics, Eq.(1) is not applicable.

For the negative S-wave scattering length between the two fermionic species, $a < 0$, in the low-density regime, $k_F \mid a \mid \ll 1$, the ground state energy per particle , $\epsilon(n)$, is well represented by an expansion in power of $k_F \mid a \mid$ [5]

$$\epsilon(n) = 2E_F[\frac{3}{10} - \frac{1}{3\pi}k_F \mid a \mid + 0.055661(k_F \mid a \mid)^2 - 0.00914(k_F \mid a \mid)^3 + ...], \tag{3}$$

where $E_F = \hbar^2 k_F^2/(2m)$.

In the opposite regime, $a \to -\infty$,the Bertsch many-body problem, $\epsilon(n)$ is proportional to that of the non-interacting Fermi gas

$$\epsilon(n) = (1+\beta)\frac{3}{10}\frac{\hbar^2 k_F^2}{m}, \tag{4}$$

where a universal parameter β [6] is estimated to be $\beta = -0.56$ [7].

In the $a \to +0$ limit the system reduces to the dilute Bose gas of dimers [8]

$$\epsilon(n) = E_F(-1/(k_F a)^2 + a_m k_F/(6\pi) + ...), \tag{5}$$

where a_m is the boson-boson scattering length. Solution of 4-fermion problem for contact scattering provided the value $a_m \approx 0.6a$ [9].

In Refs.[1,2] it has been proposed a simple interpolation of the form $\epsilon(n) \approx E_F P(k_F a)$ with a smooth function $P(x)$ mediating between the known limits.

For the negative a it has been proposed a [2/2] Padé approximant for the function $P(x)$

$$P(x) = \frac{3}{5} - 2\frac{\delta_1 \mid x \mid + \delta_2 x^2}{1 + \delta_3 \mid x \mid + \delta_4 x^2}, \tag{6}$$

where $\delta_1 = 0.106103$, $\delta_2 = 0.187515$, $\delta_3 = 2.29188$, $\delta_4 = 1.11616$. Eq.(6) is constructed to reproduce the first four terms of the expansion (3) in the low-density regime and also to reproduce exactly results of the recent Monte Carlo calculations [7], $\beta = -0.56$, in the unitary limit, $k_F a \to -\infty$.

For the positive a case (the interaction is strong enough to form bound molecules with energy E_{mol}) it has been considered a [2/2] Padé approximant

$$P(x) = \frac{E_{mol}}{2E_F} + \frac{\alpha_1 x + \alpha_2 x^2}{1 + \alpha_3 x + \alpha_4 x^2}, \tag{7}$$

where parameters α are fixed by two continuity conditions at large x, $1/x \to 0$, and by two continuity conditions at small x. For example, $\alpha_1 = 0.0316621$, $\alpha_2 = 0.0111816$, $\alpha_3 = 0.200149$, and $\alpha_4 = 0.0423545$ for $a_m = 0.6a$.

The aspect ratio, presented in Fig. 1, shows that the effect of inclusion of the OWD (quantum pressure) on the expansion of superfluid for the conditions of Ref.[6] is about 1%.

Fig. 2 and Fig. 3 show the comparison between [2/2] Padé approximations, Eqs.(6,7), and the lowest order constrained variational (LOCV) approximation [10] and the BCS mean-field theory [11] for $\epsilon(n)$. The LOCV calculations agree very well with the [2/2] Padé approximation results on the BCS side ($a < 0$). It is evident the difference between our results and the BCS mean-field theory calculations. For example, the BCS mean-field gives $\beta = -0.41$.

The predictions of Eq.(1) with $\epsilon(n)$ from Eq.(6) for the axial cloud size of strongly interacting ^6Li atoms are shown in Fig 4. It indicates that the TF approximation of the kinetic energy density is a very good approximation for the experimental conditions of Ref.[12], $N\lambda \approx 10^4$ (inclusion of the OWD gives a negligible effect, $< 0.5\%$).

In Fig. 5, we present the calculations for the frequency of the radial compression mode ω_{rad} as a function of the dimensional parameter $(N^{1/6}a/a_{ho})^{-1}$ in the case of an anisotropic trap ($\omega_x = \omega_y = \omega_\perp$, $\omega_z/\omega_\perp = \lambda$). One can easily see that the corrections to the hydrodynamic approximation (HA) (inclusion of the OWD) are important even for relatively large N and λN. For example, the correction to ω_{rad} in unitary limit is larger than 11% and 25% for $\lambda = 10^{-2}$, $N = 10^4$ and $\lambda = 10^{-2}$, $N = 10^3$, respectively.

In the HA, ω_{rad} is independent of N for a fixed $(N^{1/6}a/a_{ho})^{-1}$. The deviation from this behavior does not demonstrate the cross-over to the $1D$ behavior, since $\lambda N > 1$. It demonstrates that the validity of the HA depends on the properties of the trap. We note here that the collective modes of the Fermi gas under harmonic confinement in the framework of the hydrodynamic approximation was considered recently in [13,14].

In Fig.6, the calculated radial compressional frequency is compared with experimental data [15] in the BCS-BEC crossover region. There is a very good agreement between calculations and experimental data [15].

However our calculations for ω_{rad} disagree with experimental data of Ref.[16]. It is well known that the hydrodynamic equation is expected to be applicable for describing the macroscopic excitations of the system up to energies of the order of the energy gap, Δ, needed to break-up a Cooper pair. But for the trapped gas Δ is a function of $\vec{r}$ (Δ decreasing when we go away from the center). It is naturally to assume that condition of the applicability of

hydrodynamics to describe the macroscopic excitations of the system at $T = 0$ is

$$\frac{\hbar\Omega}{\tilde{\Delta}} \ll 1, \tag{8}$$

where Ω is the frequency of the macroscopic excitations, $\tilde{\Delta} = \int n(\vec{r})\Delta(\vec{r})d\vec{r}/N$. To calculate $\tilde{\Delta}$ we have used results of Refs.[17,18].

Fig.7 shows the comparison between the average energy gap and frequencies of the transverse and axial breathing modes. It may explain why our calculations disagree with experimental data of Ref.[16], see also Ref.[19]. Taking into account the trap difference between Ref.[15] and Ref.[16] we expect that the Duke University group will reproduce the 910G strong change in the Ω_{rad} of Ref.[16] at $B \approx 1000G$.

As for axial mode, interesting results may start at $B \approx 1250$G if ω_{ho} of the trap is about $2\pi 60$ Hz.

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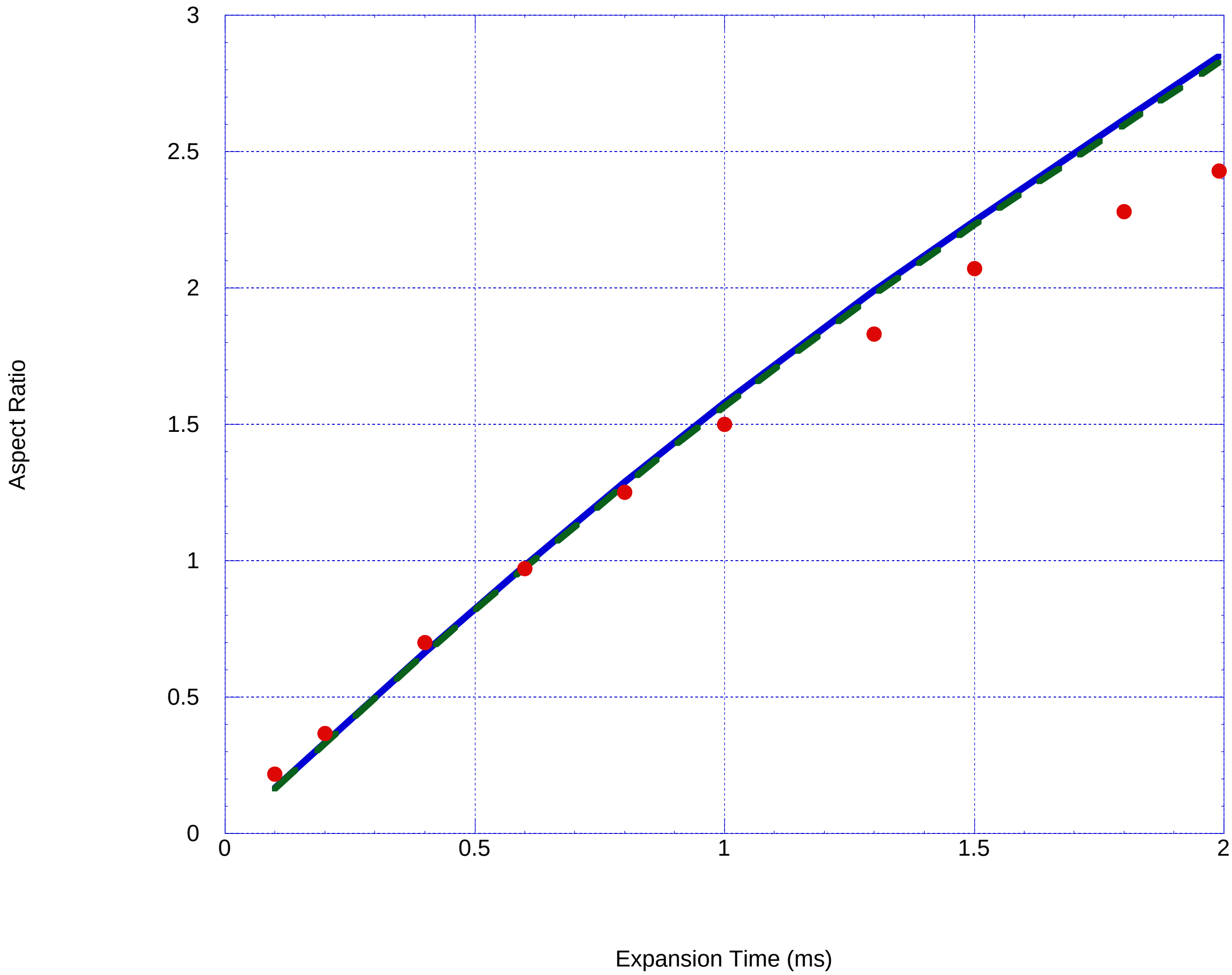

Fig. 1. Aspect ratio of the cloud of the $N = 7.5 \times 10^4\ {}^6Li$ atoms as a function of time after release from the trap ($\omega_\perp = 2\pi \times 6605$Hz, $\omega_z = 2\pi \times 230$Hz). The circular dots indicate experimental data from the Duke University group [6]. The solid line and the dashed line represent theoretical calculations in the unitary limit ($a \to -\infty$) including the quantum pressure term and in the hydrodynamic approximation, respectively.

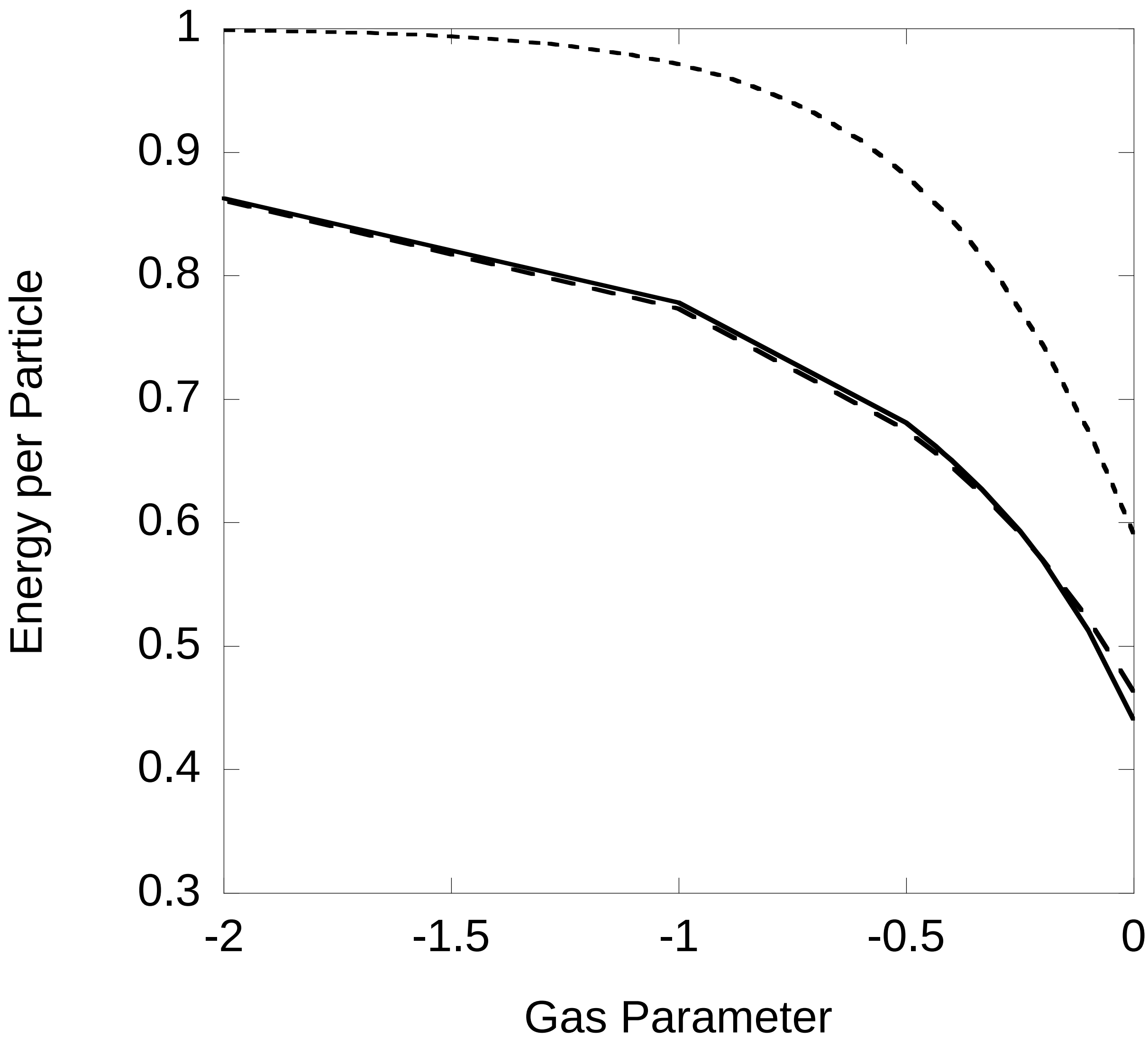

Fig.2. The ground state energy per particle, $\epsilon(n)$, in units of $3\hbar^2 k_F^2/(10m)$ as a function of the gas parameter $(k_F a)^{-1}$. The solid line, the long dashed line and the short dashed line represent the results calculated using the [2/2] Padé approximation, Eq.(6), the LOCV approximation, and the BCS mean-field theory, respectively.

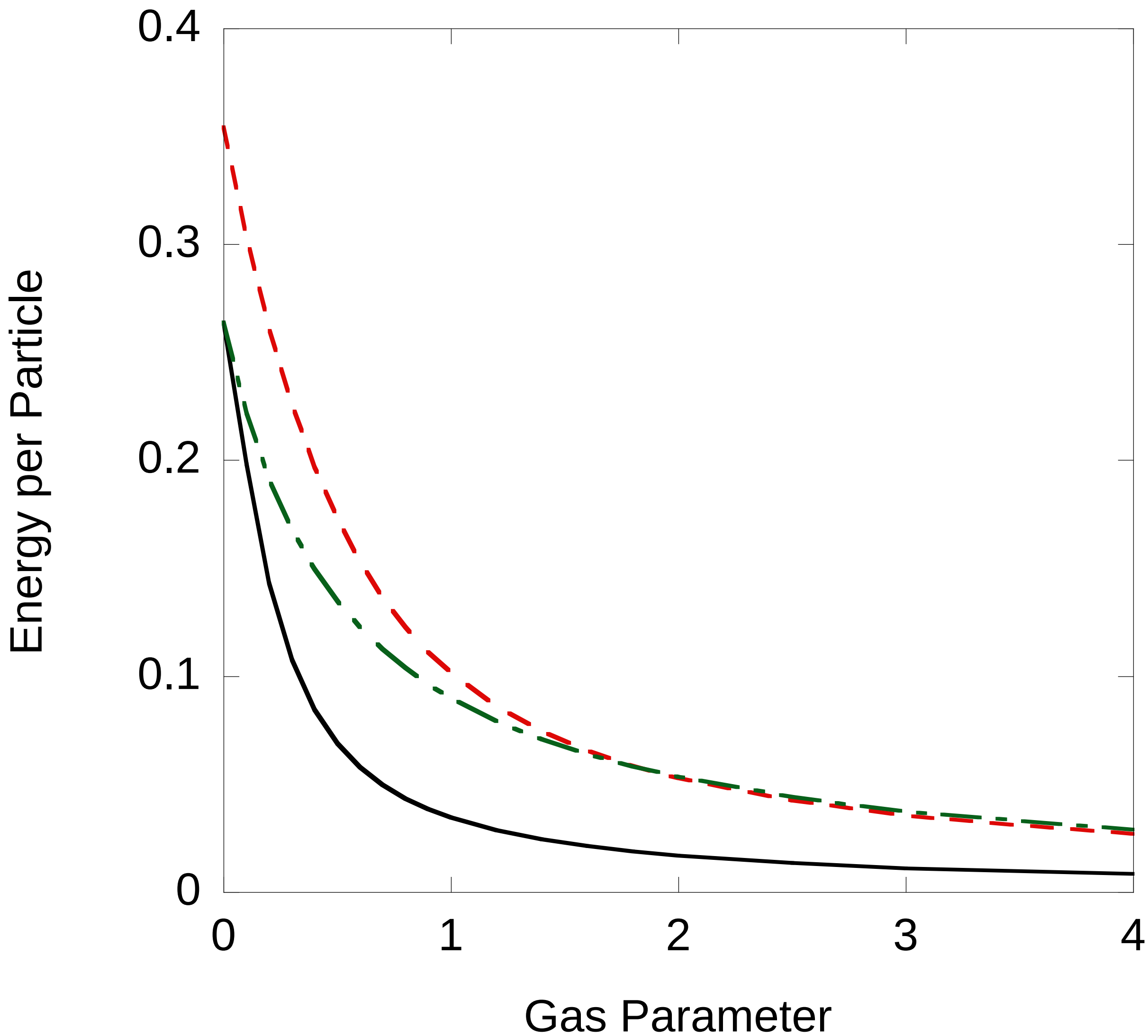

Fig.3. The ground state energy per particle, $\epsilon(n) + |E_{mol}|/2$, in units of $\hbar^2 k_F^2/(2m)$ as a function of the gas parameter $(k_F a)^{-1}$. The dashed line, the dotted-dashed line and the solid line represent the results calculated using the BCS mean-field theory, the [2/2] Padé approximation, Eq.(7), with $a_m = 2a$, and $a_m = 0.6a$, respectively.

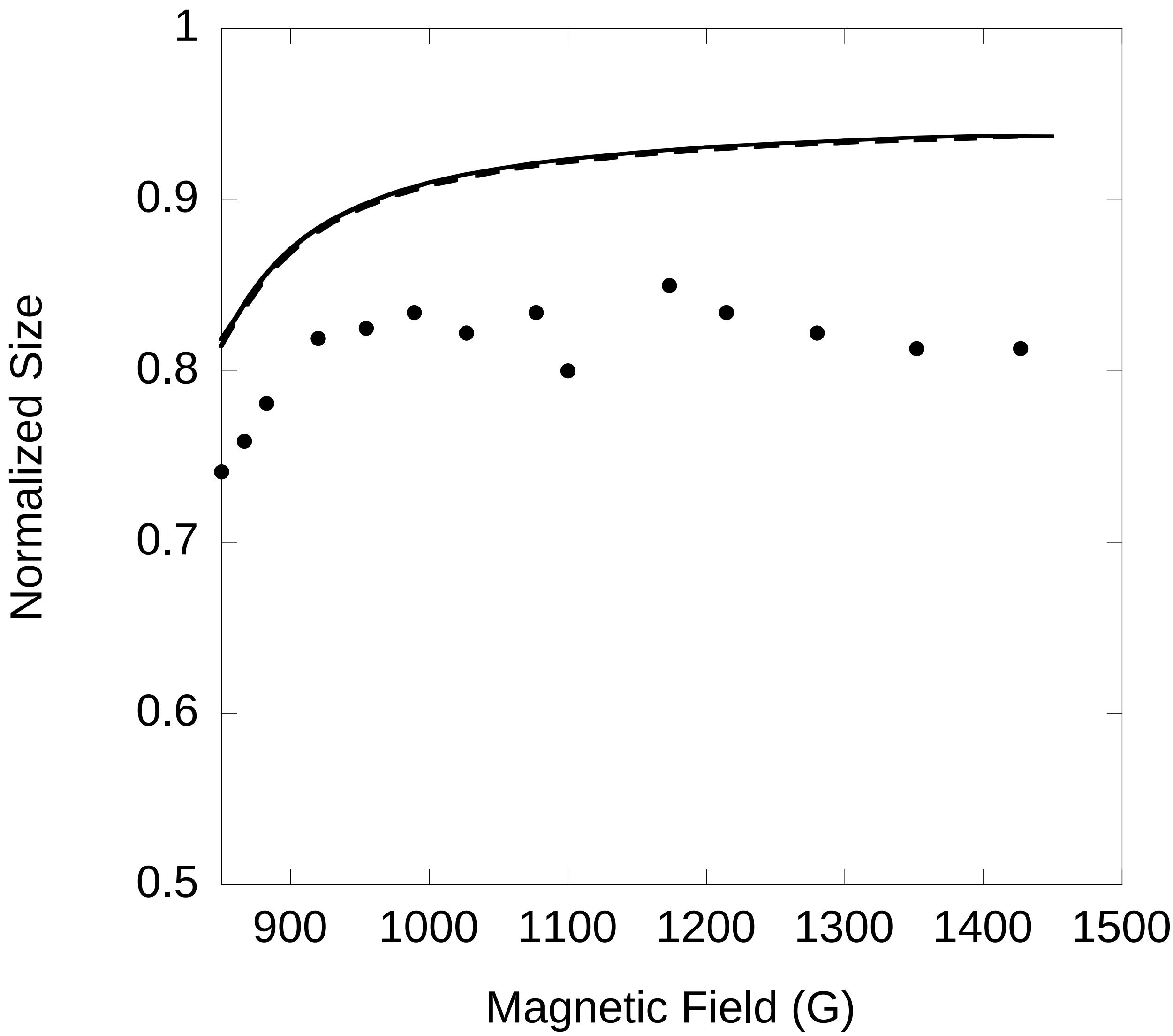

Fig. 4. Axial cloud size of strongly interacting ^6Li atoms after normalization to a non-interacting Fermi gas with $N = 4 \times 10^5$ atoms as a function of the magnetic field B. The trap parameters are $\omega_\perp = 2\pi \times 640$Hz, $\omega_z = 2\pi(600B/kG + 32)^{1/2}$Hz. The solid line and dashed line represent the results of theoretical calculation that includes the OWD or uses the TF approximation for the kinetic energy density, respectively. The circular dots indicate experimental data from the Innsbruck group [12].

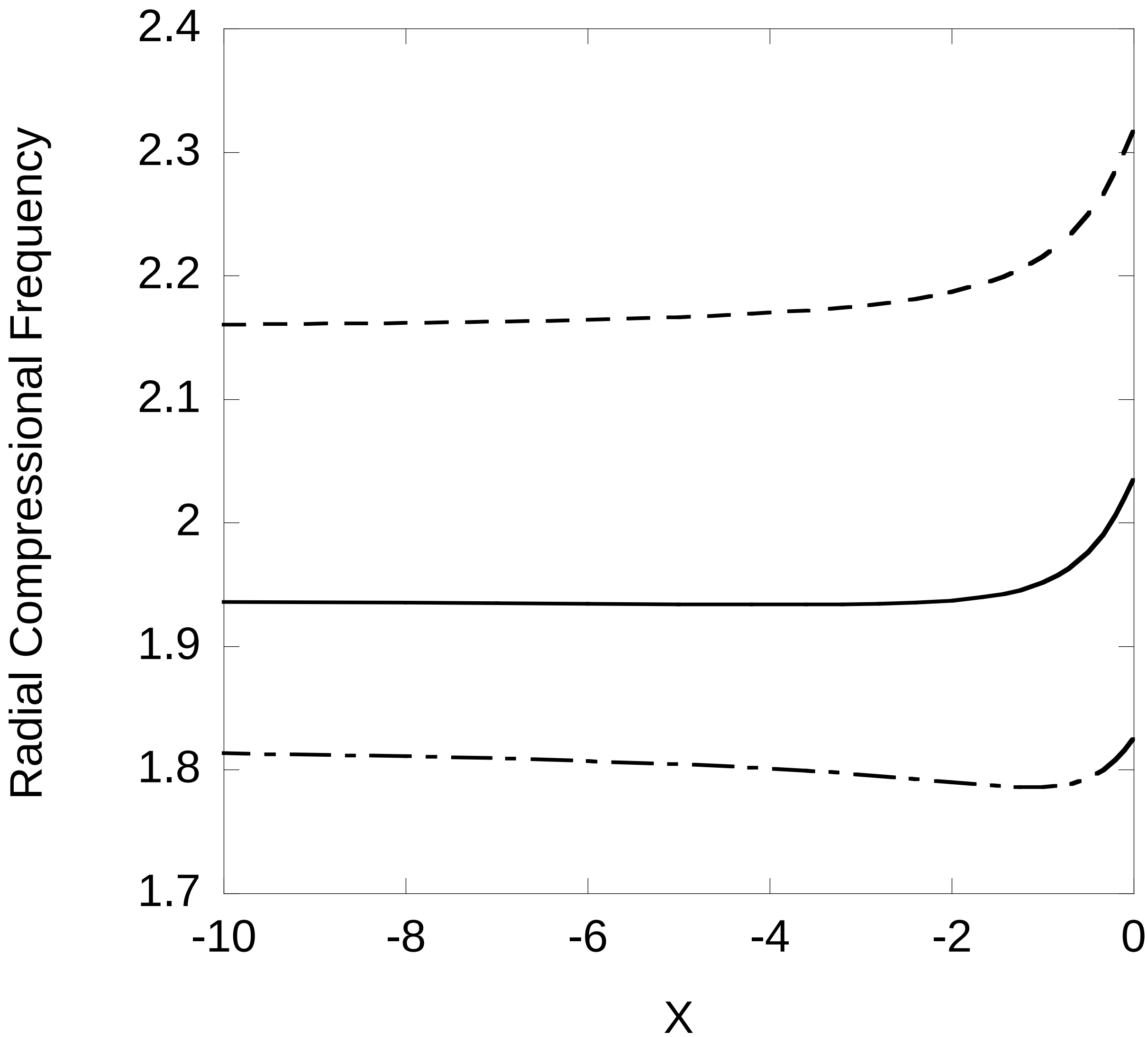

Fig. 5. Radial compressional frequency, ω_{rad}, of the cloud of the $N = 10^4$ fermions (solid line) and $N = 10^3$ fermions (dashed line) in unit of $\omega_\perp$ as a function of the dimensional parameter X=$(N^{1/6}a/a_{ho})^{-1}$. The trap parameter λ is assumed to be equal to 10^{-2}. The lower line (dashed-dotted line) represents the results in the hydrodynamic approximation, in which ω_{rad} is independent of N for a fixed $(N^{1/6}a/a_{ho})^{-1}$.

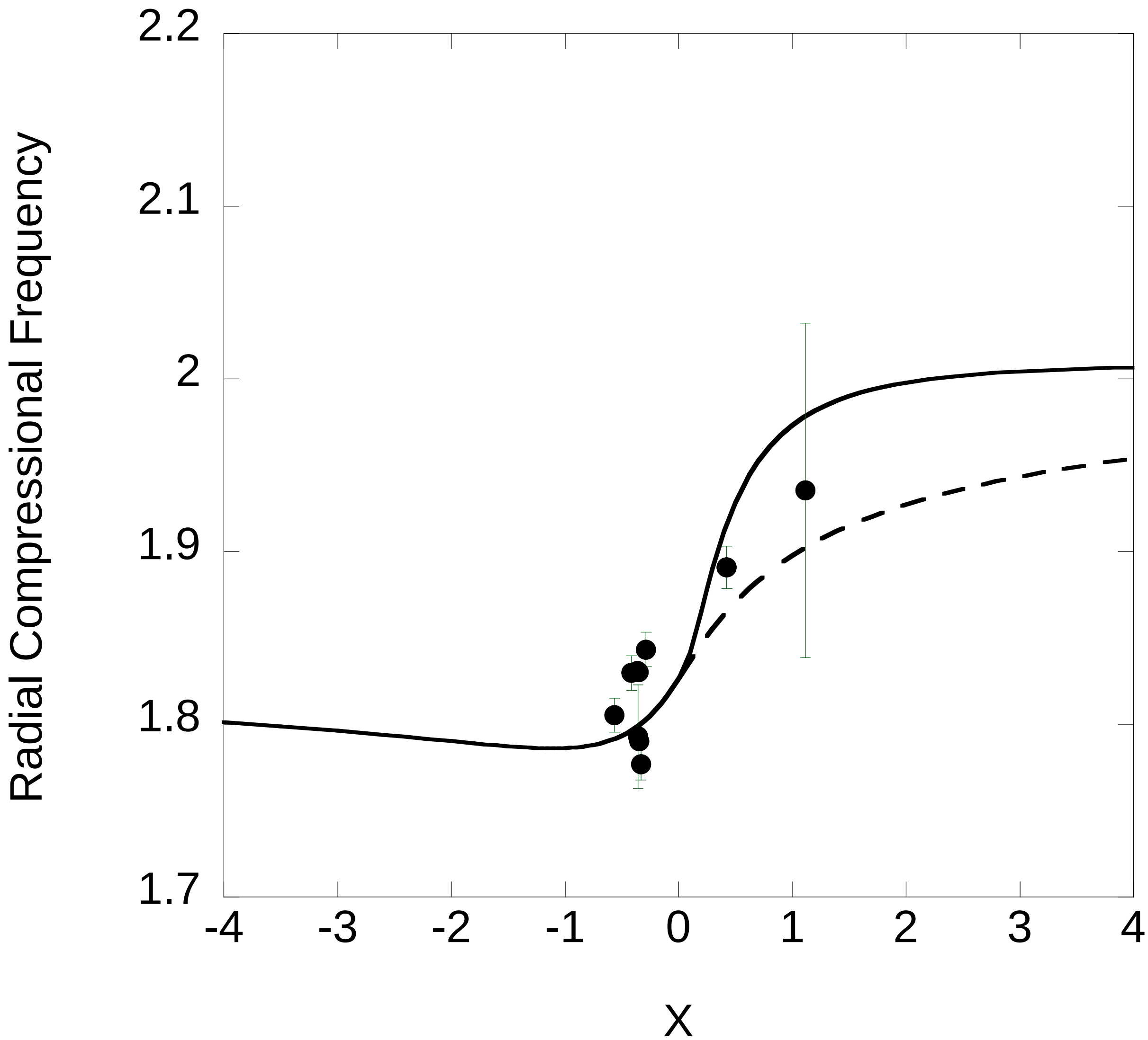

Fig.6. The radial compressional frequency as a function of X=$(N^{1/6}a/a_{ho})^{-1}$. The solid line and the dashed line represent the results calculated using the [2/2] Padé approximation with $a_m = 0.6a$ and $a_m = 2a$, respectively. The solid circles with error bars are the experimental results given by the Duke University group [15].

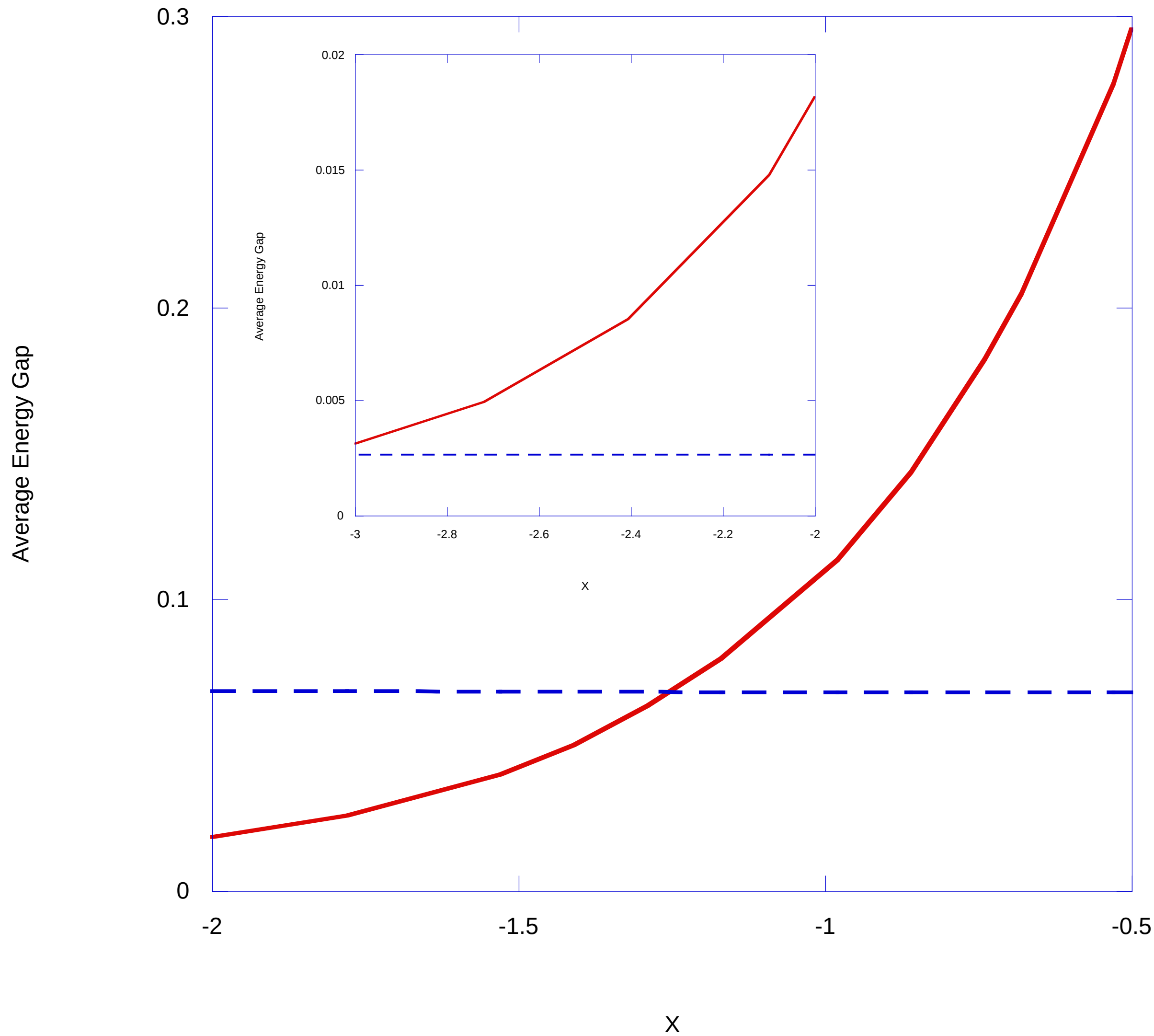

Fig.7. The average energy gap in units of $\hbar\omega_{ho}N^{1/3}$ of an elongated trapped $N = 4 \times 10^5$ Fermi atoms ($\lambda = 0.045$) as a function of the parameter $X = (k_F(0)a)^{-1}$ (solid lines). The dashed lines in the main plot and in the inset are the frequencies of the transverse and axial breathing modes in the same units ($\hbar\omega_{ho}N^{1/3}$), respectively.

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